Fundamentals of Monte Carlo simulations of radiation transport with FLUKA

20th FLUKA Beginners' Course

Stellenbosch University (South Africa)

May 28 – June 1, 2018

Overview

The radiation transport problem

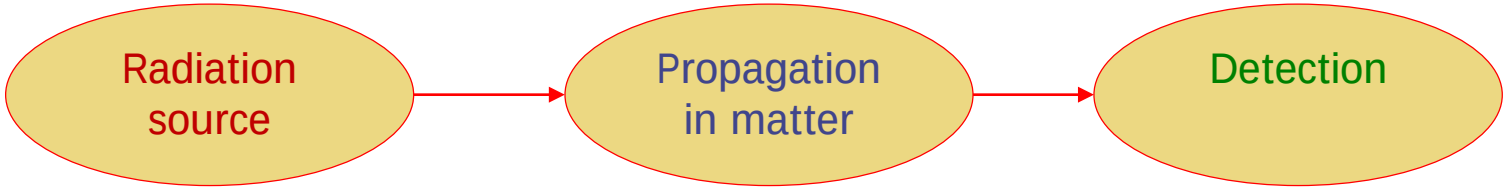
- Basic ingredients
- What equation governs the problem?
- How does one solve it?

FLUKA's approach: the Monte Carlo method

- Random variables: how to characterize and exploit them
- The Central Limit Theorem
- Basic assumptions in FLUKA as a MC code for radiation transport
- Limitations : what NOT to expect

THE RADIATION TRANSPORT PROBLEM

The radiation transport problem



Photons,
Leptons ($e^{\pm}$, $\mu^{\pm}$, $\tau^{\pm}$, ν),
Hadrons (n, p, π, Σ,…),
Heavy ions (Z,A),
Radioactive sources

Cosmic rays,
Colliding particle beams,
Synchrotron radiation

"Monoenergetic"/Spectral

Energies up to several PeV and down to few keV (thermal energies for neutrons).

Arbitrary geometry,
Various bodies,
materials, compounds.

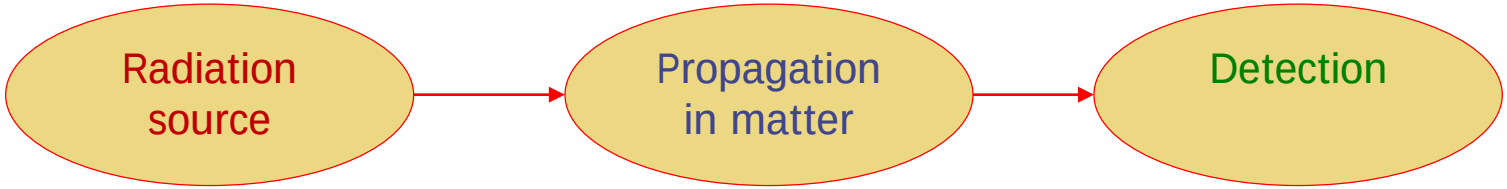
Radiation-matter interaction mechanisms,

Secondary particles,
Particle shower,
Material activation,
Magnetic fields…

Measure/estimate/score:

Energy-angle particle spectra,
Deposited energy,
Material damage,
Biological effects,
Radioactive inventories…

The radiation transport problem



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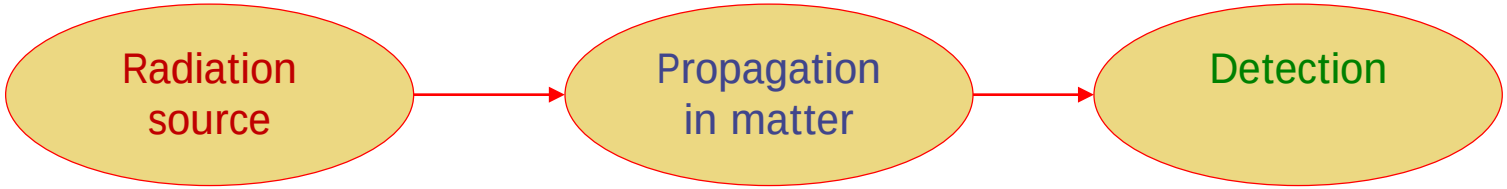
Monday afternoon

The radiation transport problem



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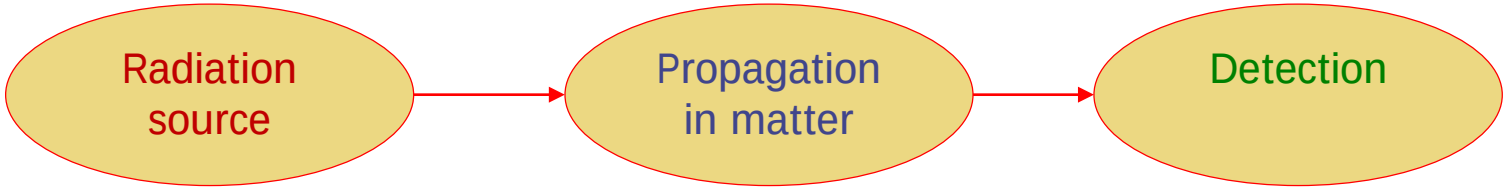
Tuesday morning

The radiation transport problem



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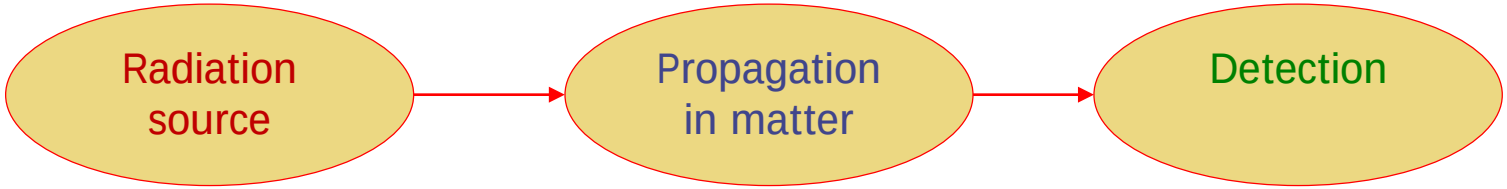
Tuesday afternoon
(hadronic interactions, scoring)

The radiation transport problem



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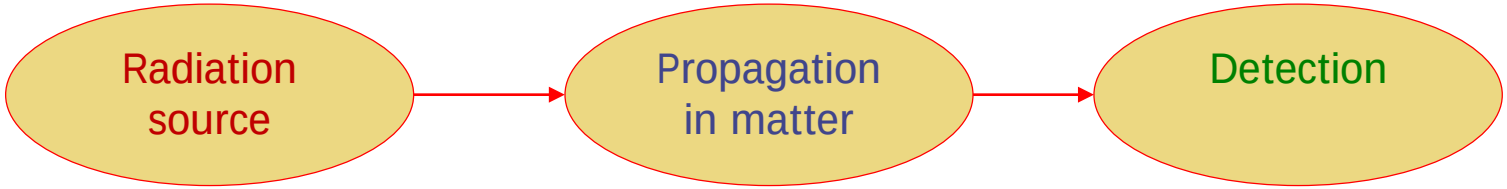
Wednesday morning (low-energy neutrons)

The radiation transport problem



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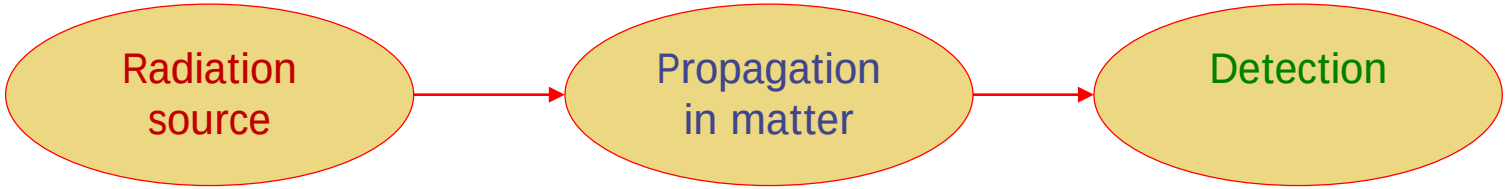
Wednesday afternoon

The radiation transport problem



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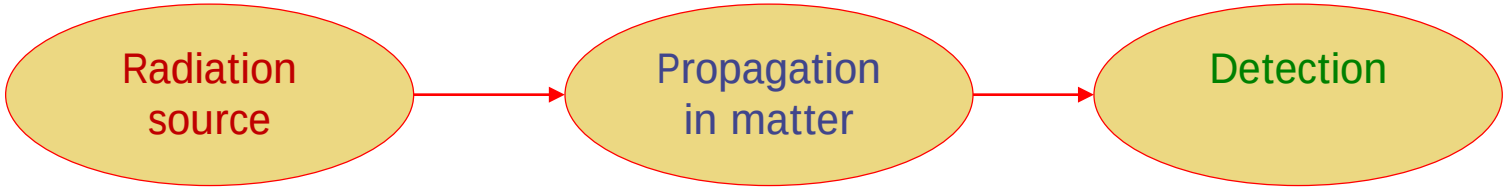
Thursday morning

The radiation transport problem



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Friday morning

The Boltzmann transport equation (1/3)

The elementary quantity to characterize how a radiation field propagates, is the number dN of transported (or generated) particles in a position within d**r** of **r**, with momentum within d**p** of **p**, at time within dt of t, given by

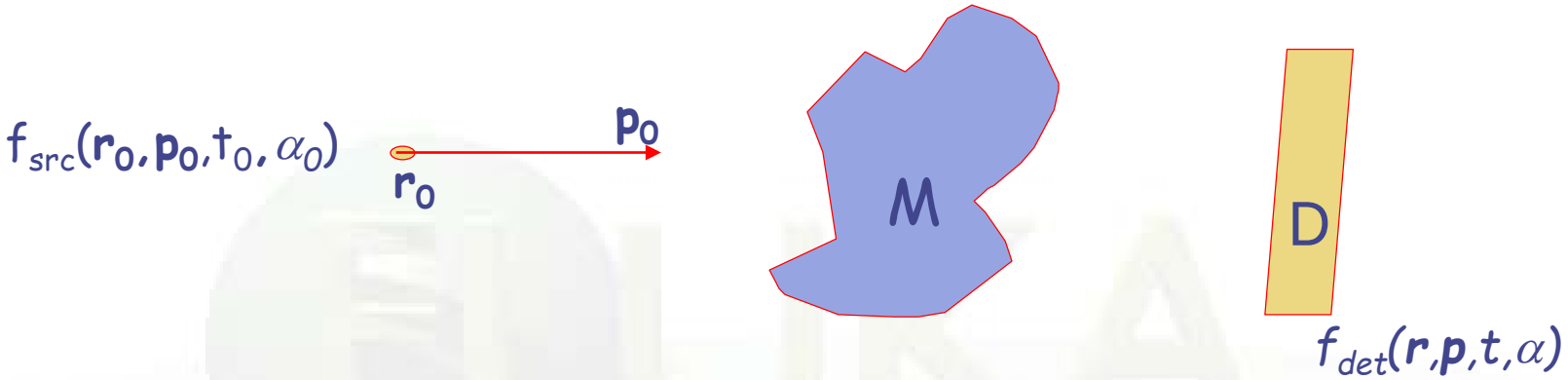
$$\mathrm{d}N = f(\mathbf{r}, \mathbf{p}, t, \alpha)\, \mathrm{d}^3\mathbf{r}\, \mathrm{d}^3\mathbf{p}\, \mathrm{d}t\, \mathrm{d}^n\alpha$$

where α includes *n* other variables (particle species, spin, etc) and $f(\mathbf{r},\mathbf{p},t,\alpha)$ is the particle-number density.

Given an initial density $f_{src}(\mathbf{r}_0,\mathbf{p}_0,t_0,\alpha_0)$, what is the particle density $f_{det}(\mathbf{r},\mathbf{p},t,\alpha)$ in a detector after propagating through a material?

The Boltzmann transport equation (2/3)

Consider a point source of, say, protons at $\mathbf{r}_0$ emitted at t_0 with momentum $\mathbf{p}_0$ traversing a material M, with a detector D after it:



For monoenergetic sources like in this case, one may write

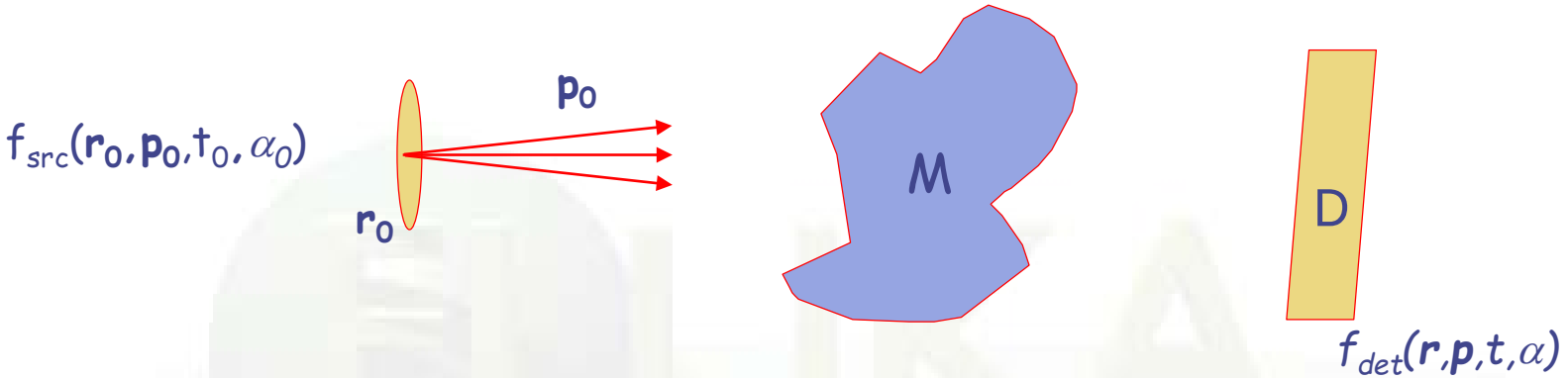
$$f_{\mathrm{det}}(\mathbf{r},\mathbf{p},t,\alpha) = G(\mathbf{r},\mathbf{p},t,\alpha;\mathbf{r}_0,\mathbf{p}_0,t_0,\alpha_0)\, f_{\mathrm{src}}(\mathbf{r}_0,\mathbf{p}_0,t_0,\alpha_0)$$

Where G(…) is a "propagator" which accounts for:

- Geometry boundary conditions
- Scattering through various interaction mechanisms
- Generation of secondary particles
- Effect of external fields (e.g. magnetic field)

The Boltzmann transport equation (3/3)

For a more general source, extended in space and with some momentum (energy) spectrum, we would have



$$f_{\mathrm{det}}(\mathbf{r}, \mathbf{p}, t, \alpha) = \int \mathrm{d}^3\mathbf{r}_0 \int \mathrm{d}^3\mathbf{p}_0 \int \mathrm{d}t_0 \int \mathrm{d}\alpha_0 \; G(\mathbf{r}, \mathbf{p}, t, \alpha; \mathbf{r}_0, \mathbf{p}_0, t_0, \alpha_0) \; f_{\mathrm{src}}(\mathbf{r}_0, \mathbf{p}_0, t_0, \alpha_0)$$

This is a very schematic formal way of writing the **Boltzmann transport equation**, in general a multi-dimensional (>6) integro-differential equation.

(See additional slides for a more detailed discussion)

Method of solution

$$f_{\rm det}(\mathbf{r},\mathbf{p},t,\alpha) = \int \mathrm{d}^3\mathbf{r}_0 \int \mathrm{d}^3\mathbf{p}_0 \int \mathrm{d}t_0 \int \mathrm{d}\alpha_0 \; G(\mathbf{r},\mathbf{p},t,\alpha;\mathbf{r}_0,\mathbf{p}_0,t_0,\alpha_0)\; f_{\rm src}(\mathbf{r}_0,\mathbf{p}_0,t_0,\alpha_0)$$

Unfortunately, general analytical or closed-form solutions are out of reach*.

We need an effective (and efficient!) numerical scheme

A fruitful path consists in resorting to stochastic methods.

Before showing the main idea: we review the minimum required toolkit of statistics/probability concepts.

*R. Oswald, *J. Electr Spectr Relat Phen* **61** 251 (1993).

PROBABILITY AND STATISTICS TOOLKIT

Random variables

A random variable X describes the outcome of an experiment whose value we cannot predict with certainty. But nevertheless we know:

- Its possible values: X in $[x_{min}, x_{max}]$.
- How likely each value of X is.

Random variables can be

- discrete, e.g., throw of a die, number of energy losses in a step…
- continuous, e.g., energy or angle of a photon traversing a slab

Randomness itself can be

- Intrinsic: e.g. quantum processes.
- Extrinsic: e.g. in the throw of a six-sided fair die.

Probability density functions

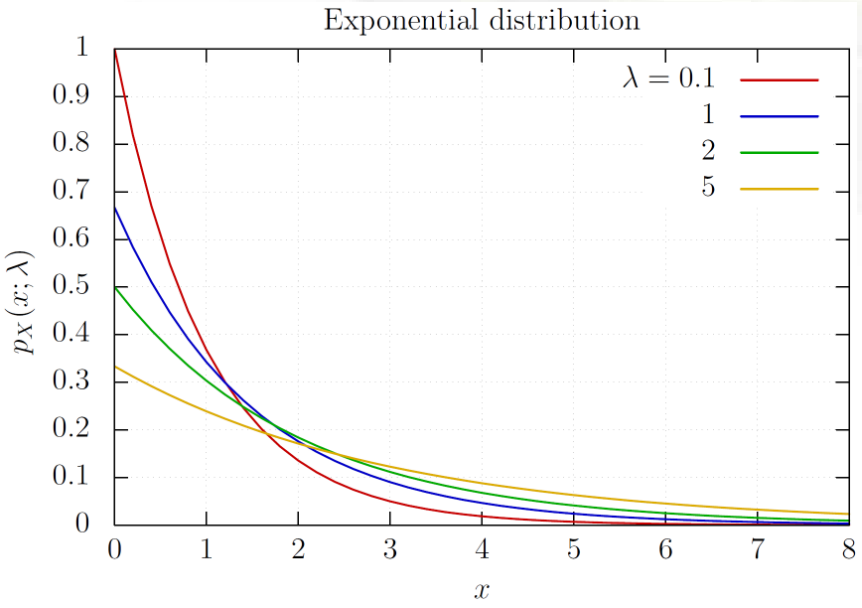
The probability density function p(x) describes the likelihood of a given value of x. p(x) should be:

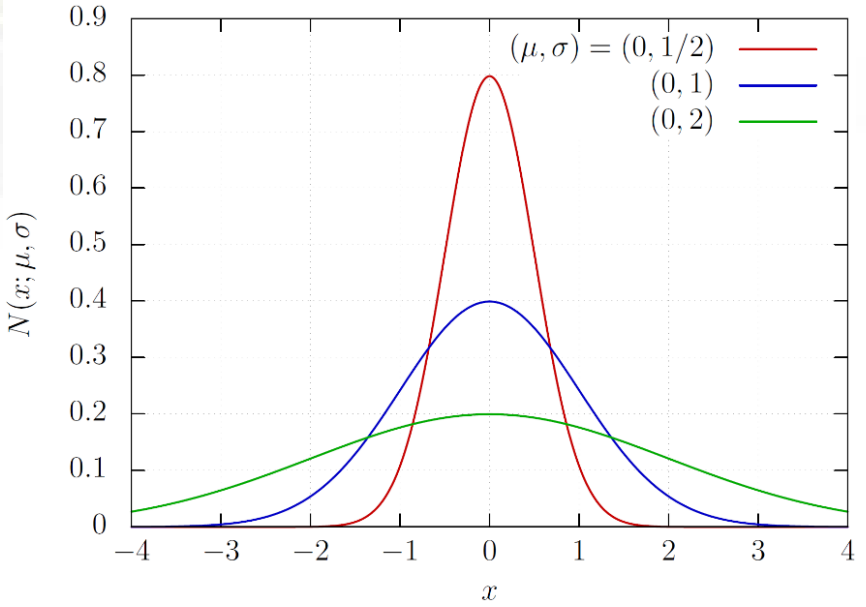
- Normalized: $\int dx\, p(x) = 1$
- Non-negative: $p(x) >= 0$ for any x.
- Probability of x in [a,b]: $\int_a^b dx\, p(x)$

Examples:

$$p(x;\lambda) = \frac{1}{\lambda} e^{-x/\lambda}$$

$$p(x;\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/(2\sigma^2)}$$





Mean and standard deviation

* If X~p(x), the mean or expectation value of X is obtained by integrating x weighted by p(x) over the whole domain of X:

$$\langle X \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \; x p(x)$$

Examples:
Gaussian: <X> = … = μ,
Exponential: <X> = … = λ .

* The standard deviation is a measure of the spread of p(x) around <X>. Its square, the variance, is given by:

$$\sigma^2 = \langle (X - \langle X \rangle)^2 \rangle = \ldots = \langle X \rangle^2 - \langle X^2 \rangle$$

Examples

Gaussian: σ^2 = … = σ^2 (Note: σ is not FWHM)
Exponential: σ^2 = … = λ^2

Expectation value of f(x)

- If X~p(x), the expectation value of f(X) is obtained by integrating f(x) weighted by p(x) over the whole domain of X:

$$\langle f(X) \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \; f(x) p(x)$$

If $X_1, X_2, \ldots, X_n$ follow $p(x_1, x_2, \ldots, x_n)$, we have a multi-dimensional integral:

$$\langle f(X_1, X_2, \ldots) \rangle = \int_{-\infty}^{\infty} \mathrm{d}x_1 \int_{-\infty}^{\infty} \mathrm{d}x_2 \; \ldots f(x_1, x_2, \ldots) p(x_1, x_2, \ldots)$$

Recalling our schematic way of writing the transport equation,

$$f_{\mathrm{det}}(\mathbf{r}, \mathbf{p}, t, \alpha) = \int \mathrm{d}^3\mathbf{r}_0 \int \mathrm{d}^3\mathbf{p}_0 \int \mathrm{d}t_0 \int \mathrm{d}\alpha_0 \; G(\mathbf{r}, \mathbf{p}, t, \alpha; \mathbf{r}_0, \mathbf{p}_0, t_0, \alpha_0) \; f_{\mathrm{src}}(\mathbf{r}_0, \mathbf{p}_0, t_0, \alpha_0)$$

we can **formally** read this multi-dimensional integral as an expectation value of a non-trivial function according to a probability density function governing the radiation transport process.

Central Limit Theorem

Still we do not know how to evaluate the integral efficiently. The Central Limit Theorem provides the needed foundation.

If $x_1, x_2, \ldots, x_n$ are n values of X sampled from a PDF p(x) with mean $\langle X \rangle = \mu$ and standard deviation σ, the Central Limit Theorem states that

$$Y = \frac{1}{n}\sum_{i=1}^{n} X_i$$

is a random variable following a Gaussian distribution with mean $\langle Y \rangle = \mu$ and standard deviation $\sigma/\sqrt{n}$.

Thus, **in the limit of large n (many samples), $\langle Y \rangle = \langle X \rangle$**. As an extension,

$$Z = \frac{1}{n}\sum_{i=1}^{n} f(X_i)$$

is a random variable following a Gaussian distribution with mean $\langle Z \rangle = \langle f(x) \rangle$ and standard deviation $\sigma \sim 1/\sqrt{n}$.

THE MONTE CARLO METHOD

MC Mathematical foundation

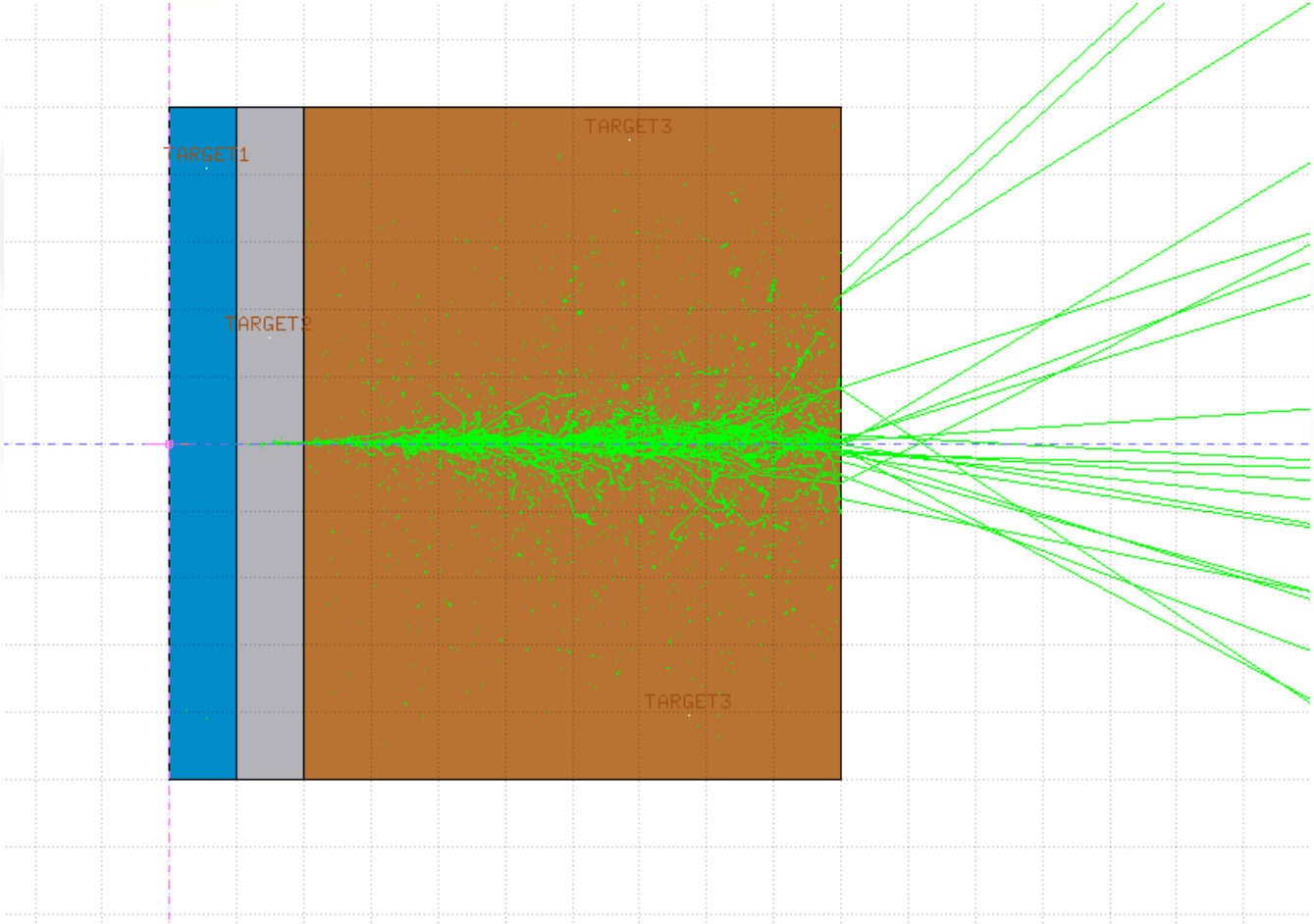
The Central Limit Theorem provides the mathematical foundation of the Monte Carlo method:

> Given any physical observable *A*, that can be expressed as the result of a convolution of random processes, the average value of *A* can be obtained by sampling many values of *A* according to the probability distributions of the random processes.

MC is indeed an integration method that allows to efficiently evaluate multi-dimensional integrals by sampling from a suitable probability density.

Radiation transport a la Monte Carlo

One can estimate physical observables by sampling an ensemble of particle trajectories (random walk) according to given interaction cross sections.

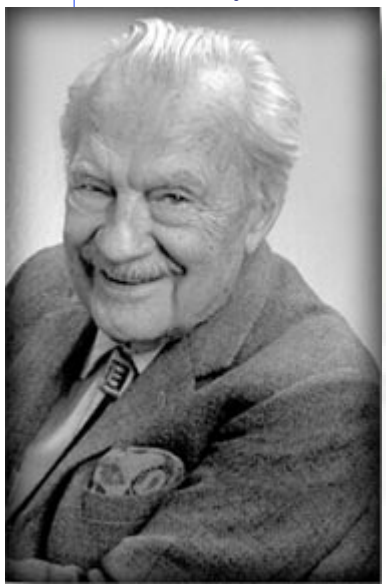


Integration efficiency

- Traditional numerical integration methods (e.g., Simpson) converge to the true value as $N^{-1/n}$, where N = number of "points" (intervals) and n = number of dimensions
- Monte Carlo converges as $N^{-1/2}$, **regardless of the number of dimensions**
- Therefore:
  - $n = 1$ ➔ MC is not convenient
  - $n = 2$ ➔ MC is about equivalent to traditional methods
  - $n > 2$ ➔ MC converges faster (and the more so the greater the dimensions)
- With the integro-differential Boltzmann equation the dimensions are the 7 of phase space, but we use the integral form: the dimensions are those of the largest number of "collisions" per history (the Neumann term of highest order)
- Note that the term "collision" comes from low-energy neutron/photon transport theory. Here it should be understood in the extended meaning of "interaction where the particle changes its direction and/or energy, or produces new particles"

The Monte Carlo method for radiation transport problems

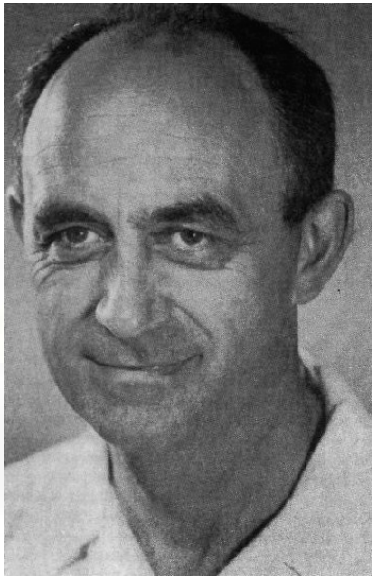
Developed by John von Neumann, Stanislaw Ulam and Nicholas Metropolis (who gave it its name), and independently by Enrico Fermi



N. Metropolis

S. Ulam

J. von Neumann



E. Fermi

Ref:
N. Metropolis, "The beginning of the Monte Carlo method", *Los Alamos Science Special Issue* 125-130 (1987)

Analog Monte Carlo simulation

- For radiation transport problems, the Monte Carlo model (random walk of particles through a medium according to given interaction cross sections) is a faithful reproduction of the actual physical process (restrictions apply; see below).

- Such an approach (analog Monte Carlo) is a simulation technique, since every step of the model corresponds to an identical step in the simulated process

- Anticipate: biasing (lecture on Wednesday).

SAMPLING

(Pseudo)random numbers

- The basic tool for all Monte Carlo integrations are random numbers, i.e. values of a random variable following a given probability density.
- In the real world: random outcomes of physical processes (intrinsic randomness), e.g. *https://en.wikipedia.org/wiki//dev/random*
- In computer world: pseudo-random numbers. Pseudo-random numbers (PRN) are sequences that follow the uniform distribution, constructed from deterministic algorithms (PRN generators).
- The basic pdf is the uniform distribution:

$$f(\xi) = 1 \quad 0 \le \xi < 1$$

- PRN generators start from one or several seeds to generate sequences.

- Families of pseudo-random number generators:
  - Linear congruence: $X_{n+1} = mod(a\, X_n + c, m)$, carefully chosen a, c, m
  - Lagged Fibonacci generator: $X_{n+1} = mod(X_{n-p} @ X_{n-q}, m)$, @ is +,-,...

Refs: Marsaglia G. et al., Stat Probabil. Lett. **66** 183-187 (2004)
Stat Probabil. Lett. **8** 35-39 (1990)

Random-number generator state in FLUKA output

```
NEXT SEEDS:    2F3F4        0        0        0        0        0   181CD     3039        0        0
         6                        94                        94              1.1433840E-02          1.0000000E+30                  12

NEXT SEEDS:    8FBBF        0        0        0        0        0   181CD     3039        0        0
         8                        92                        92              9.0010017E-03          1.0000000E+30                  12
```

*out and *err

ran* file content:

```
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14842CCE3FD618F9
```

RANDOMIZ WHAT(1) iniSeed

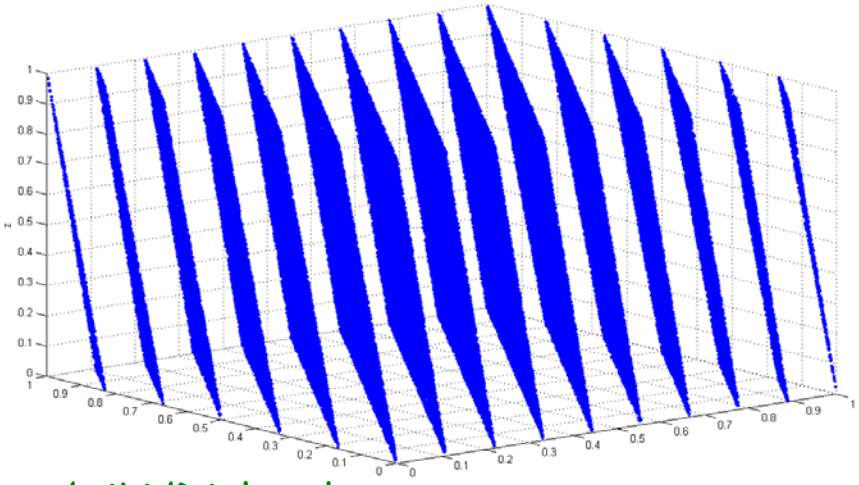
(Pseudo)random numbers

- PRN generators have a period, after which the sequence is identically repeated. However, a repeated number does not imply that the end of the period has been reached. Some available generators have periods $>10^{61}$

- A PRN sequence looks random but it is not: it can be successfully tested* for statistical randomness although it is generated deterministically

- A pseudo-random process is easier to produce than a really random one, and has the advantage that it can be reproduced exactly

The infamous RANDU, used from the 60s to the 80s, purged by the 90s (poor choice of parameters)
https://en.wikipedia.org/wiki/RANDU



Refs:

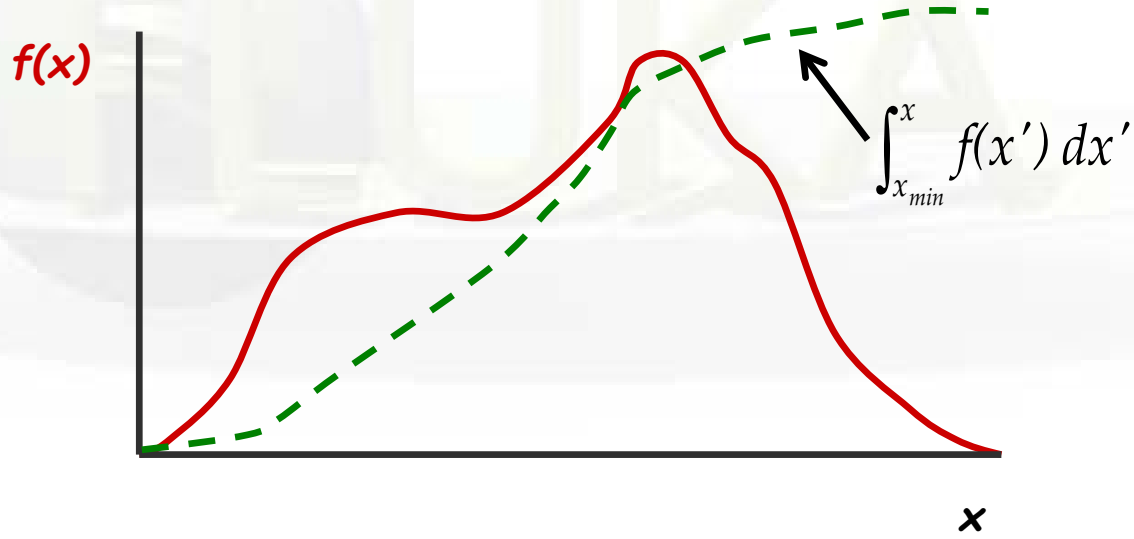
* Diehard battery of tests: https://en.wikipedia.org/wiki/Diehard_tests

- Donald Knuth, *The art of computer programming, Vol II, Chap 3*

Random sampling: the key to Monte Carlo

The central problem of the Monte Carlo method:

Given a Probability Density Function (pdf), ***f(x)***, generate samples of ***x***'s distributed according to ***f(x)*** (***x*** can be multidimensional)



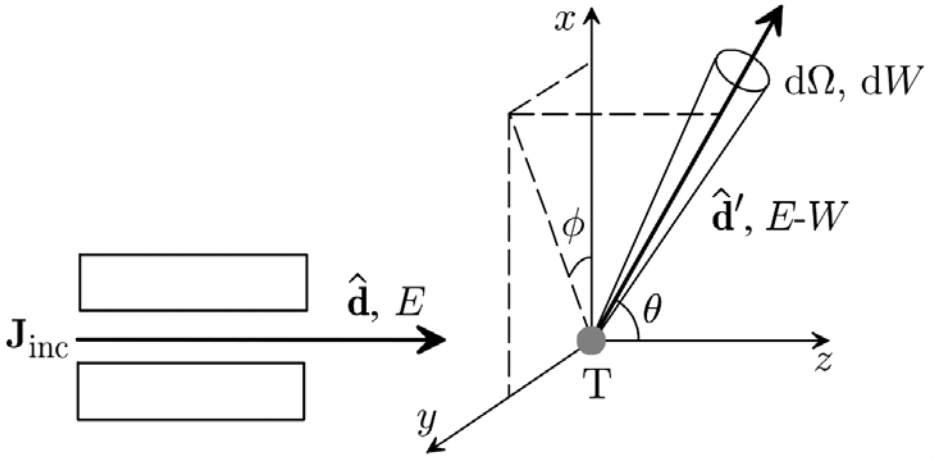
(See extra material for more details on sampling techniques)

WHAT DO WE SAMPLE FROM IN A MC SIMULATION?

INTERACTION CROSS SECTION AND MEAN FREE PATH

Interaction cross section

For each interaction mechanism, there exists a differential cross section $d\sigma / (d\Omega\ dW)$ which describes the probability for the projectile particle to be scattered within $d\Omega$ of Ω, and/or to lose an energy within dW of W:



The total cross section

$$\sigma(E, Z, A) = \int_{4\pi} d\Omega \int dW \frac{d\sigma}{d\Omega dW}$$

is a measure of the probability for the incoming particle to undergo the considered type of interaction. It can be interpreted as the cross sectional area of the target.

EM processes $\sigma \sim 10^3$ barn, nuclear processes $\sigma \sim 1$ barn.

(1barn = 10^{-24}cm^2).

The mean free path and its distribution

Consider n particles per unit time and unit surface impinging perpendicularly on a thin material slab of width ds with a density of N scattering centers per unit volume, each having a cross sectional area σ.

The number of lost particles is $dn = n N\sigma\, ds$.
The interaction probability in ds is: $dn/n = N\sigma\, ds$
Let p(s) be the distribution of path lengths to the next interaction.

Probability that next interaction is within ds of s:

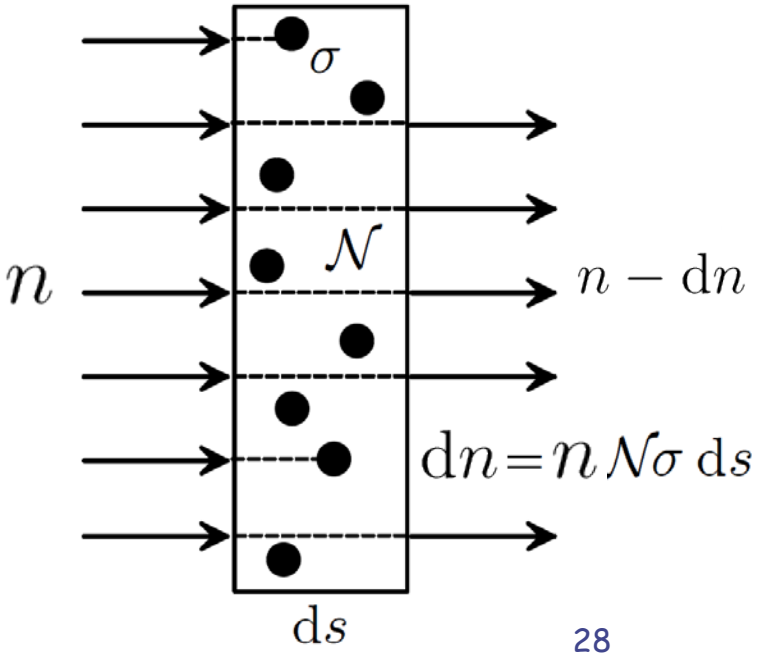
$$p(s) = [\, 1 - \int_0^s ds'\, p(s') \,]\ (N\sigma)$$
$$= \int_s^{inf} p(s')\,(N\sigma)\, ds'$$

The solution of this diff eq is

$$p(s) = (N\sigma)\, e^{-s(N\sigma)}$$

An exponential distribution!
Expectation value of s:

$\langle s \rangle = 1/(N\sigma) = \lambda$, the mean free path.



Several interaction mechanisms

If several interaction mechanisms are available, the total interaction cross section is obtained by addition (no interference between processes)

$$\sigma = \sum_{i=1}^{n} \sigma_i$$

The total mean free path is given by

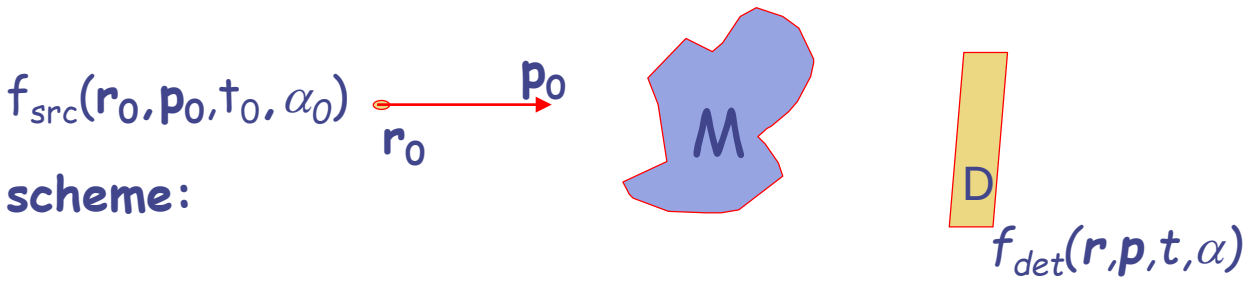
$$\lambda_t = \frac{1}{\mathcal{N}\sigma}$$

That is,

$$\lambda_t^{-1} = \mathcal{N} \sum_{i=1}^{n} \sigma_i = \sum_{i=1}^{n} \lambda_i^{-1}$$

LOGICAL FLOW OF A MONTE CARLO SIMULATION OF RADIATION TRANSPORT

Particle transport Monte Carlo



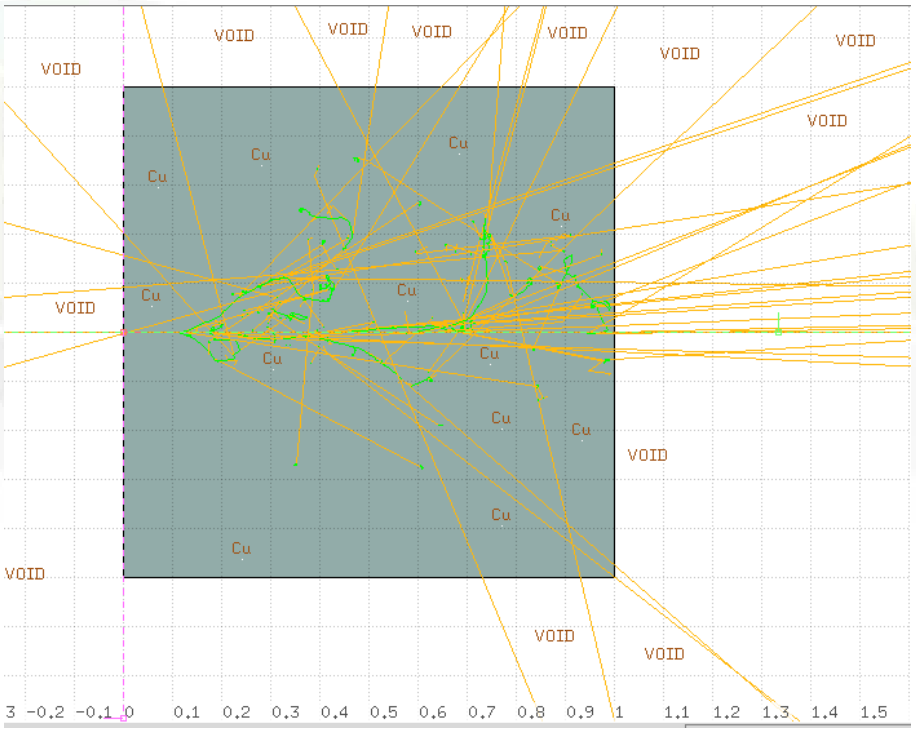
General (simplified) scheme:

1. Initialize particle position and momentum (or energy+direction).
   1.1 If particle is in vacuum, bring it to next material boundary.
2. Determine total cross section at current energy, material, etc: σ
3. *Sample step length to next interaction from exponential distribution.*
4. *Decide nature of interaction:* $P_i = \sigma_i / \sigma, \quad i=1,2,\ldots,n$
5. *Sample energy loss (or change of direction) from differential cross section for interaction mechanism i.*
6. *Add generated secondary particles to the stack* if any.*
7. *Go to 2 unless*
   1. *Particle energy drops below user preset threshold (lecture Thu)*
   2. *Particle exits the geometry*

Radiation transport a la Monte Carlo

10 trajectories, 50-MeV photons on 1 cm Cu

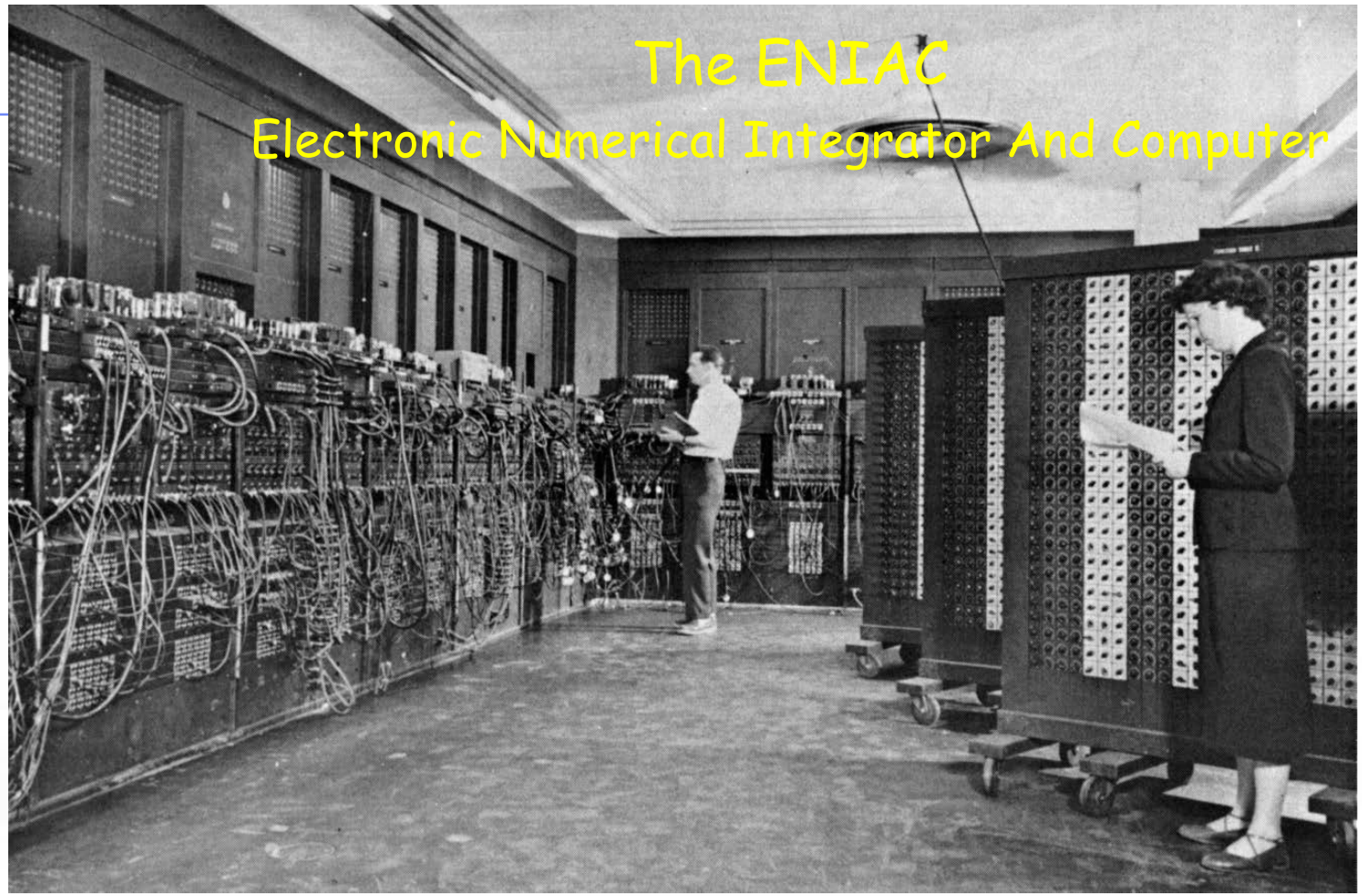
Orange: photons,
Green: electrons



Feasible with present-day computers, but…

The ENIAC

Electronic Numerical Integrator And Computer



"It had a speed on the order of one thousand times faster than that of electro-mechanical machines; this computational power, coupled with general-purpose programmability, excited scientists and industrialists alike. This combination of speed and programmability allowed for thousands more calculations for problems, as ENIAC calculated a trajectory that took a human 20 hours in 30 seconds (a 2400× increase in speed)" (wiki)

ASSUMPTIONS AND LIMITATIONS

Assumptions made by most MC codes:

- Static, homogeneous, isotropic, amorphous media and geometry
  Problems: e.g. moving targets*, atmosphere must be represented by discrete layers of uniform density, radioactive decay may take place in a geometry different from that in which the radionuclides were produced*.

  * These restrictions have been mostly overcome in FLUKA
- Markovian process: the fate of a particle depends only on its actual present properties, not on previous events or histories
- Particles do not interact with each other
  Problem: e.g. the Chudakov effect (charges cancelling in e^+e^- pairs)
- Particles interact with individual electrons / atoms / nuclei / molecules
  Problem: invalid at low energies (X-ray mirrors), see next slide
- Material properties are not affected by particle reactions
  Problem: e.g. burnup

Validity of the trajectory picture

In a MC simulation, we follow particle trajectories.

Heisenberg uncertainty principle: one can strictly NOT determine position and momentum with arbitrary resolution.

Under certain circumstances, the particle picture is nevertheless a sufficiently good approximation.

Wave/particle duality → Every particle has an associated de-Broglie wavelength:

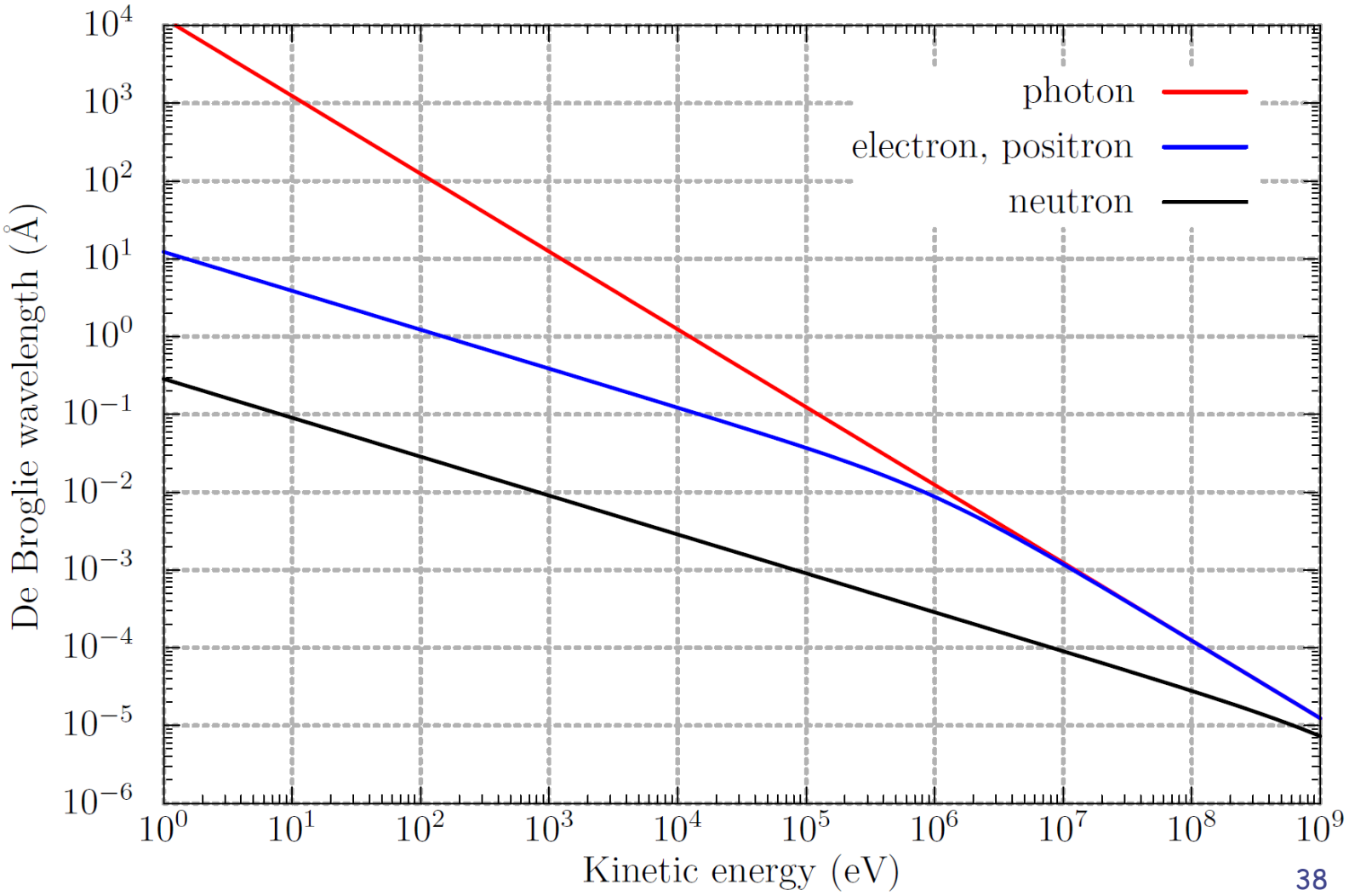
$$\lambda_{\mathrm{dB}} = \frac{hc}{\sqrt{E_K(E_K + 2m_0c^2)}}$$

Particle/trajectory picture is fine, provided that the **de-Broglie wavelength is small compared to typical obstacle distances**, e.g. interatomic distances (of the order of a few Angstroem).

https://en.wikipedia.org/wiki/Wave%E2%80%93particle_duality

Validity of the trajectory picture

De-Broglie wavelength: $$\lambda_{\mathrm{dB}} = \frac{hc}{\sqrt{E_K(E_K + 2m_0c^2)}}$$



STATISTICAL UNCERTAINTY IN MC SIMULATIONS

From the slide on central limit theorem

Given any physical observable Z, that can be expressed as the result of a convolution of random processes, the average value of Z can be obtained by sampling many (n) values of Z according to the probability distributions of the random processes.

We recall

$$Z = \frac{1}{n}\sum_{i=1}^{n} f(X_i)$$

is a random variable following a Gaussian distribution with mean <Z>=<f(x)> and standard deviation σ ~1/sqrt(n).

Thus, the precision of a MC estimator depends on the number of samples:

$$\sigma \propto \frac{1}{\sqrt{N}}$$

i.e., for twice as good a precision, we need ~4 times as many samples

Statistical Errors:

- Can be calculated for single histories, or for batches of several histories
- Distribution of scoring contributions by single histories can be very asymmetric (many histories contribute little or zero)
- The standard deviation of an estimator calculated from batches or from single histories is an estimate of the standard deviation of the actual distribution ("error of the mean")
- How good is such an estimate depends on the type of estimator and on the particular problem (but it converges to the true value for $N \rightarrow \infty$)

Statistical Errors

- The variance of the mean of an estimated quantity **x** (e.g., fluence), calculated in N batches, is:

$$\sigma^2_{<x>} = \frac{1}{N-1}\left[\frac{\sum_1^N n_i x_i^2}{n} - \left(\frac{\sum_1^N n_i x_i}{n}\right)^2\right]$$

mean of squares – square of means

N – 1

where:

n_i = number of histories in the i^{th} batch

$n = \Sigma n_i$ = total number of histories in the N batches

x_i = average of x in the i^{th} batch: $x_i = \sum_{j=1}^{n_i} \frac{x_{ij}}{n_i}$

where x_{ij} is the contribution to x of the j^{th} history in the i^{th} batch

In the limit $N = n$ and $n_i = 1$, the expression applies to single history statistics

Statistical Errors

Practical tips:

- Use always at least 5-10 batches of comparable size (it is not at all mandatory that they be of equal size)
- Never forget that the variance itself is a stochastic variable subject to fluctuations
- Be careful about the way convergence is achieved: often (particularly with biasing) apparently good statistics with few isolated spikes could point to a lack of sampling of the most relevant phase-space part
- Plot 2D and 3D distributions! In those cases the eye is the best tool in judging the quality of the result

Statistical errors, systematic errors, and… mistakes

Statistical errors, due to sampling (in)efficiency

Relative error	Quality of Tally *(from an old version of the MCNP Manual)*
50 to 100%	Garbage
20 to 50%	Factor of a few
10 to 20	Questionable
< 10%	Generally reliable

- The MCNP guideline is empirically based on experience, not on a mathematical proof. But it has been generally confirmed also working with other codes
- Small penetrations and cracks are very difficult to handle by MC, because the "detector" is too small and too few non-zero contributions can be sampled, even by biasing

OTHER SOURCES OF UNCERTAINTY

Statistical errors, systematic errors, and... mistakes

- Apart from the statistical uncertainty, systematic errors may affect the accuracy of MC results at various instances:
  - Adopted physics model: different codes are based on different physics models. Some models are better than others. Some models are better in a certain energy range. Model quality is best shown by benchmarks at the microscopic level (e.g. thin targets)
  - Transport algorithm: due to imperfect algorithms, e.g., energy deposited in the middle of a step*, inaccurate path length correction for multiple scattering*, missing correction for cross section and *dE/dx* change over a step*, etc. Algorithm quality is best shown by benchmarks at the macroscopic level (thick targets, complex geometries)
  - Cross-section data uncertainty: an error of 10% in the absorption cross section can lead to an error of a factor 2.8 in the effectiveness of a thick shielding wall (10 attenuation lengths). Results can never be better than allowed by available experimental data!

* Not in FLUKA!

Statistical errors, systematic errors, and… mistakes

Systematic errors, due incomplete knowledge

- Missing information:
  - material composition not always well known. E.g. concrete/soil composition (how much water content? Can be critical)
  - beam losses: most of the time these can only be guessed. Close interaction with engineers and designers is needed
  - presence of additional material, not well defined (cables, supports…)
  - Is it worth to do a very detailed simulation when some parameters are unknown or badly known?

Systematic errors, due to simplification

- Geometries that cannot be reproduced exactly (or would require too much effort)
- Air contains humidity and pollutants, has a density variable with pressure

Statistical errors, systematic errors, and… mistakes

Code mistakes ("bugs")

- MC codes can contain bugs:
  - Physics bugs: e.g. pair production cross sections fitted by a polynomial, oscillating instead of saturating at high energies, non-uniform azimuthal scattering distributions, energy non-conservation…
  - Programming bugs (as in any other software, of course)

User mistakes

- mis-typing the input: Flair is excellent at checking, but the final responsibility is on the user
- error in user code: use the built-in features as much as possible!
- wrong units
- wrong normalization: quite common
- unfair biasing: energy/space cuts cannot be avoided, but must be done with much care
- forgetting to check whether gamma production is available in the neutron cross sections (e.g. Ba cross sections)

ANALOGUE VS BIASED MONTE CARLO

Analog Monte Carlo

In an analog Monte Carlo calculation, not only the mean of the contributions converges to the mean of the actual distribution, but also the variance and all moments of higher order:

$$\lim_{N \to \infty} \left[\frac{\sum_1^N \left(x - \bar{x} \right)^n}{N} \right]^{\frac{1}{n}} = \sigma_n$$

Then, partial distributions, fluctuations and correlations are all faithfully reproduced: in this case (and in this case only!) we have a real simulation

Brief anticipation of biasing

- In many cases, it is more efficient to replace the actual process by a different one resulting in the same average values but built by sampling from modified distributions
- Such a *biased process*, if based on mathematically correct variance reduction techniques, converges to the same expectation values as the unbiased one
- But it cannot provide information about the higher moments of statistical distributions (fluctuations and correlations)
- In addition, the faster convergence in some user-privileged regions of phase space is compensated by a slower convergence elsewhere

See biasing lecture.

Summary

The radiation transport problem

- Basic ingredients
- What equation governs the problem?
- How difficult is it to solve?

FLUKA's approach: the Monte Carlo method

- Random variables: how to characterize and exploit them
- The Central Limit Theorem
- Basic assumptions in FLUKA as a MC code for radiation transport
- Limitations : what NOT to expect

END

Extra slides

Phase space:

- Phase space: a concept of classical Statistical Mechanics
- Each Phase Space dimension corresponds to a particle degree of freedom
- 3 dimensions correspond to Position in (real) space: x, y, z
- 3 dimensions correspond to Momentum: p_x, p_y, p_z
  (or Energy and direction: E, θ, φ)
- More dimensions may be envisaged, corresponding to other possible degrees of freedom, such as quantum numbers: spin, etc.
- Another degree of freedom is the particle type itself (e^-, p,γ..)
- Time can also be considered as a coordinate, or it can be considered as an independent variable
- Each particle is represented by a point in phase space
- The number of particles in an infinitesimal phase-space region is

$$dN = f(x, p, t, \alpha) d^3p d^3x dt d^n\alpha$$

- Where *f* is a probability density function (α=extra degrees)

Particle Transport

- Particle transport is represented by the evolution of $f(x,p,t,\alpha)$ due to transport, scattering, external forces, particle production, particle absorption/decay
- The most general description of particle transport is the Boltzmann equation, an integro-differential equation based on balance in phase space
- Any solution of the Boltzmann equation needs the definition of a Source and one or more Detectors :
- The source provides the intitial particle distribution function in a given phase space region, the detector is a phase space region where the modified $f(x,p,t,\alpha)$ is to be calculated
- In general:

$$f(x,p,\alpha) = \iiint G(x,p,\alpha,x',p',\alpha') f_0(x',p',\alpha') d^3p' d^3x' d^n\alpha'$$

- Where G is a multi-dimensional operator that encompasses all the microscopic processes

Particle Transport

- For our discussion here, three concepts have to be retained:

1. The solution of any particle transport problem is a multi-dimensional integral
2. Particle transport is a stochastic problem, where all quantities and processes are described by probability distributions
3. The "solution" or "estimator" will again be the integral of the particle distribution function over the phase space region of interest:

$$N = \int\int\int_{\Delta p \Delta x \Lambda \alpha} f(x, p, \alpha) d^3 p d^3 x d^n \alpha$$

Another way to solve

- The solution of the Boltzmann equation involves complex integrations in many variables
- Particle non-conserving terms have also to be introduced
- Non-homogeneities of the problem further increase the complexity
- “Direct” numerical solutions can become prohibitive
- Another way to solve the transport equation is the Monte Carlo method:

Instead of INTEGRATING the probability functions, SAMPLE randomly from these distribution

- The mathematical foundation of the Monte Carlo method is in the Central limit theorem:

Mean of a distribution (1)

- In one dimension:

  Given a variable *x*, distributed according to a function *f(x)*, the mean or average of another function of the same variable *A(x)* over an interval [a,b] is given by:

$$\overline{A} = \frac{\int_a^b A(x) f(x) dx}{\int_a^b f(x) dx}$$

Or, introducing the normalized distribution f' :

$$f'(x) = \frac{f(x)}{\int_a^b f(x) dx}$$

$$\overline{A} = \int_a^b A(x) f'(x) dx$$

A special case is that of $A(x) = x$: $\overline{x} = \int_a^b x f'(x) dx$

Mean of a distribution (2)

- In several dimensions:

Given *n* variables *x,y,z,...* distributed according to the (normalized) functions *f'(x), g'(y), h'(z)...*, the mean or average of a function of those variables *A(x,y,z)* over an *n*-dimensional domain D is given by:

$$\overline{A} = \int_x \int_y \int_z \ldots \int_n A(x, y, z, \ldots)\ f'(x)\ g'(x)\ h'(x) \ldots dx\ dy\ dz \ldots$$

Often impossible to calculate with traditional methods, but we can sample N values of *A* with probability f'·g'·h'...and divide the sum of the sampled values by N:

$$S_N = \frac{\sum_1^N A(x, y, z, \ldots)}{N}$$

Each term of the sum is distributed like *A* (Analog Monte Carlo)
In this case the integration is also a simulation!

Central Limit theorem

Central limit theorem:

$$\lim_{N\to\infty} P(S_N) = \frac{1}{\sqrt{\frac{2\pi}{N}}\sigma_A} e^{-\frac{(S_N-\overline{A})^2}{2\sigma_A^2/N}}$$

For large values of N, the distribution of averages (normalized sums S_N) of N independent random variables identically distributed (according to any distribution with mean and variance ≠ ∞) tends to a normal distribution with mean $\overline{A}$ and variance σ_A^2/N

$$\lim_{N\to\infty} S_N = \lim_{N\to\infty} \frac{\sum_1^N A(x,\, y,\, z,\ldots)\, f'(x)\; g'(y)\; h'(z)\ldots}{N} = \overline{A}$$

Particle transport Monte Carlo

Application of Monte Carlo to particle transport and interaction:

- Each particle is followed on its path through matter
- At each step the occurrence and outcome of interactions are decided by random selection from the appropriate probability distributions (stochastic process).
- All the secondaries issued from the same primary are stored in a "stack" or "bank" and are transported before a new history is started
- The accuracy and reliability of a Monte Carlo depend on the models or data on which the probability distribution functions are based
- Statistical precision of results depends on the number of "histories"
- Statistical convergence can be accelerated by "biasing" techniques.

Complexity

- Simple example: a uniform monochromatic beam attenuated by a uniform shielding layer of thickness *T*
- The source term: a *flux* $\Psi(E, \theta, r) = dN/d\Omega/dE/dS = C\ \delta(E-E_0)\ \delta(\theta-\theta_0)$
- Suppose that the particle are absorbed according to a macroscopic absorption cross section Σ_t = interaction probability per cm $= \sigma_t N_A \rho/A$
- In an infinitesimal thickness *dt* the probability to be absorbed is $P = \Sigma\, dt$
- $d\Psi(t) = -\Psi(t)P = -\Psi(t)\,\Sigma_t\, dt$
- $\Psi(s) = \int_0^T \Psi(t) \exp(-\Sigma_t S)\, dt$: an *eq.* that is solved by the exponential function ➔
- $\Psi(T) = \Psi(0) \exp(-\Sigma_t T)$ EASY !!
- Now .. Suppose that the particles are not absorbed, but scattered according to some energy-dependent $d\sigma(E, \theta)/d\Omega$, exiting with $E' = g(E,\theta)$ where *g* is defined by the kinematics.
- $d\Psi(E', \theta') = \int(\Psi(E, \theta, s)\, N_A\rho/A\, d\sigma(E, \theta'')/d\Omega)\, d\theta\, dE$ where $\theta'' = \theta''-\theta$ in 3d
- $\Psi(T, E, \theta) = \int d\Psi(E', \theta') = \ldots$
- Now..suppose that the original beam was not monochromatic, or that particles can also be produced..or that the geometry is not uniform and the dimensions of the integral will explode .

The angular flux Ψ

The angular flux Ψ is the most general radiometric quantity:

particle phase space density × velocity

or also

derivative of fluence Φ(x,y,z) with respect to 3 phase space coordinates: time, energy and direction vector

$$\Psi = \frac{\partial \Phi}{\partial t \, \partial E \, \partial \vec{\Omega}} = \dot{\Phi}_{E\vec{\Omega}}$$

Ψ is fully differential, but most Monte Carlo estimators integrate it over one or more (or all) phase space dimensions: coordinates, time, energy, angle

Fluence Φ, on the opposite, is the most integral radiometric quantity:

$$\Phi = \iiint_{E\vec{\Omega}t} \dot{\Phi}_{E\vec{\Omega}} \, dE \, d\vec{\Omega} \, dt = nvt$$

where *n* = particle density in normal space, *v* = velocity, *t* = time

Particle Transport

- Particle transport == evolution of the phase space densities due to deterministic and stochastic processes
- Most general solution: Boltzmann equation: integro-differential balance equation in phase space
- The “solution” needs the definition of a source and a detector
- The “source will be a known distribution in phase space (i.e. a particle beam, or a volume filled with γ emitters..)
- The detector will be a region in phase space where we look for a solution. For instance, the neutron fluence after a shielding layer
- The transport from the source to the detector is defined by the combined probability of production and destruction processes: scattering, decay, absorption, particle production...

The Boltzmann Equation

- All particle transport calculations are (explicit or implicit) attempts to solve the Boltzmann Equation
- It is a balance equation in phase space: at any phase space point, the increment of angular flux Ψ in an infinitesimal phase space volume is equal to

sum of all "production terms"
minus
sum of all "destruction terms"

- Production:
  Sources, Translational motion "in", "Inscattering", Particle Production, Decay "in"
- Destruction:
  Absorption, Translational motion "out", "Outscattering", Decay "out"

(For convenience, we merge into a single term Particle Production and Decay "in" and in a similar way we put together Absorption and Decay "out")

The Boltzmann Equation

$$\frac{1}{v}\frac{\partial}{\partial t}\Psi(\vec{r},\vec{\Omega},E,t) + \vec{\Omega}\cdot\nabla\Psi + \Sigma_t\Psi - S = \iint \Psi(\vec{r},\vec{\Omega},E,t)\Sigma_s(\vec{r},\vec{\Omega}'\rightarrow\vec{\Omega},E'\rightarrow E)dE'd\vec{\Omega}'$$

time dependent — translation — absorption — source — scattering

Σ_t = total macroscopic cross section = interaction probability per cm

$= 1/\lambda_t = \sigma_t N_A \rho / A$

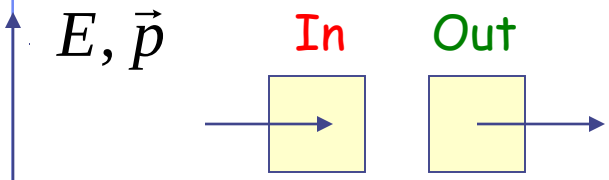
λ_t = interaction mean free path σ_t = interaction probability per atom/cm^2

Σ_s = scattering macroscopic cross section = $\sigma_s N_A \rho / A$

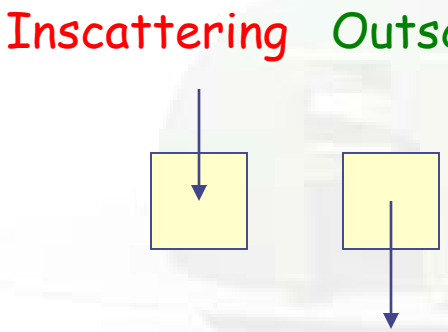
This equation is in integro-differential form. But in Monte Carlo it is more convenient to put it into integral form, carrying out the integration over all possible particle histories.

A theorem of statistical mechanics, the Ergodic Theorem, says that the average of a function along the trajectories is equal to the average over all phase space. The trajectories "fill" all the available phase space.

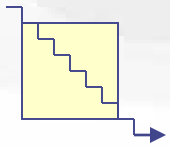
Visualizing a 2-D phase space...



Translational motion: change of position, no change of energy and direction



Scattering: no change of position, change of energy and direction



dE/dx: change of position and energy (translation plus many small scatterings

No arrows upwards! (except for thermal neutrons)

The sources and the detectors

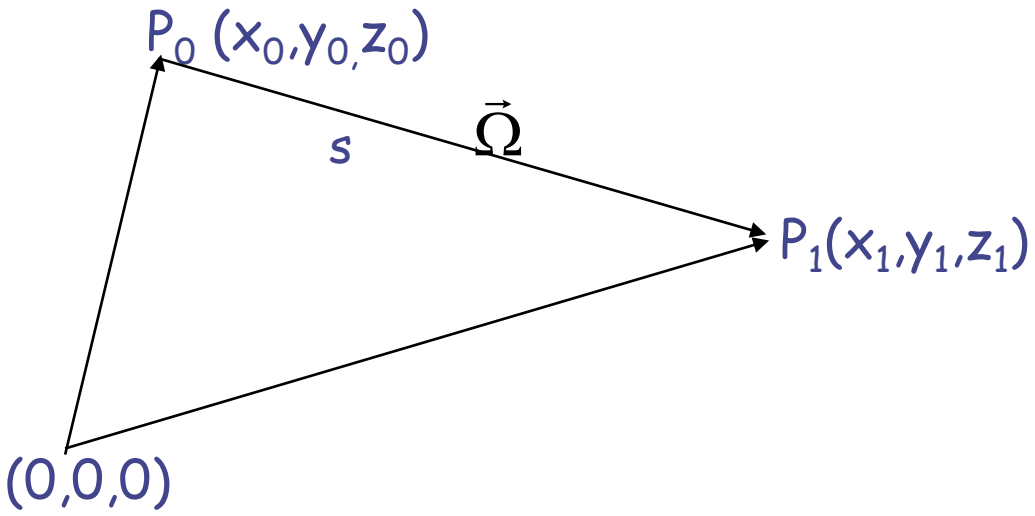
- To solve the Boltzmann Equation, we must define one or more source and one or more detectors
- A source is a region of phase space: one or more particle types, a range of space coordinates, a distribution in angle, energy and time (but often the source is simply a monoenergetic monodirectional point source — a "beam"!)
- Also a detector is a region of phase space, in which we want to find a solution of the Boltzmann equation
- We can look for solutions of different type:
  - at a number of (real or phase) space points
  - averages over (real or phase) space regions
  - projected on selected phase space hyperplanes
  - time-dependent or stationary
  - .....
- For each solution we must define a detector

Integration? Or simulation?

Why, then, is MC often considered a simulation technique?

- Originally, the Monte Carlo method was not a simulation method, but a device to solve a multidimensional integro-differential equation by building a stochastic process such that some parameters of the resulting distributions would satisfy that equation
- The equation itself did not necessarily refer to a physical process, and if it did, that process was not necessarily stochastic

Line integration of the Boltzmann Equation



Let's change coordinates along the line s in direction Ω:

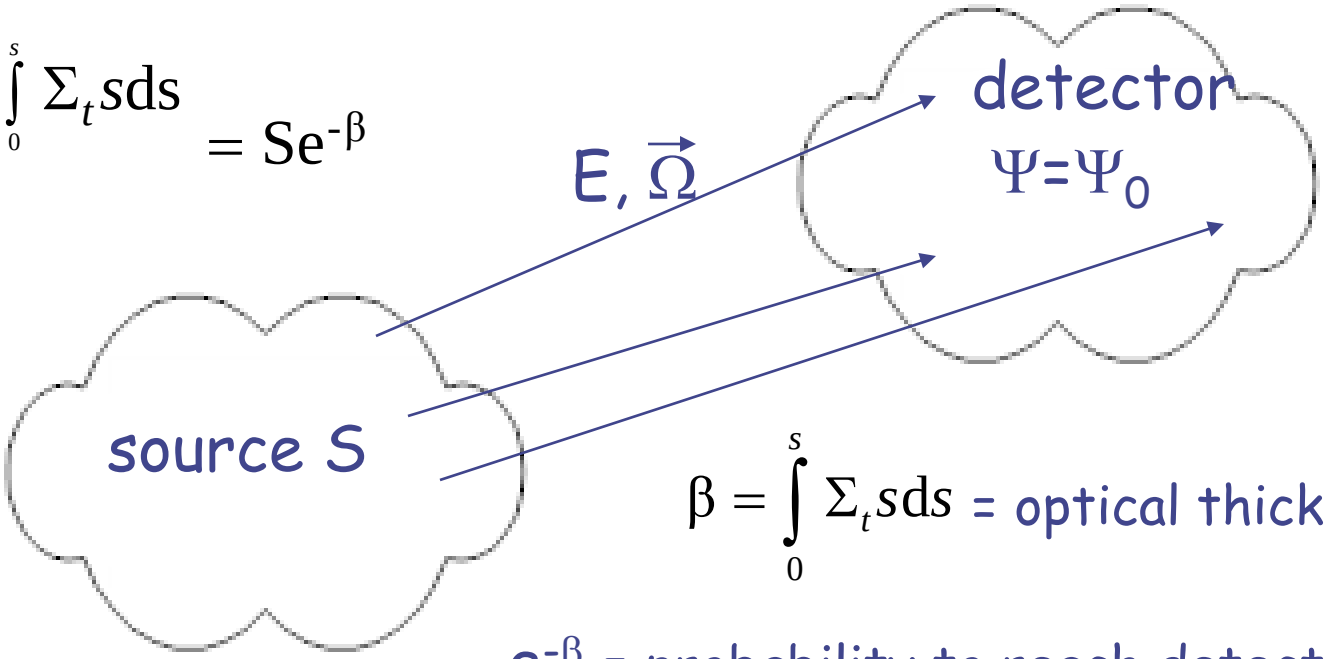
$$\frac{1}{v}\frac{\partial \Psi}{\partial t} + \frac{\mathrm{d}\Psi}{\mathrm{d}s} + \Sigma_t \Psi = S + q$$

where q indicates the scattering integral

From source to detector without interaction

uncollided term Ψ_0

$$\Psi_0 = Se^{-\int_0^s \Sigma_t s ds} = Se^{-\beta}$$



$$\beta = \int_0^s \Sigma_t s ds$$ = optical thickness

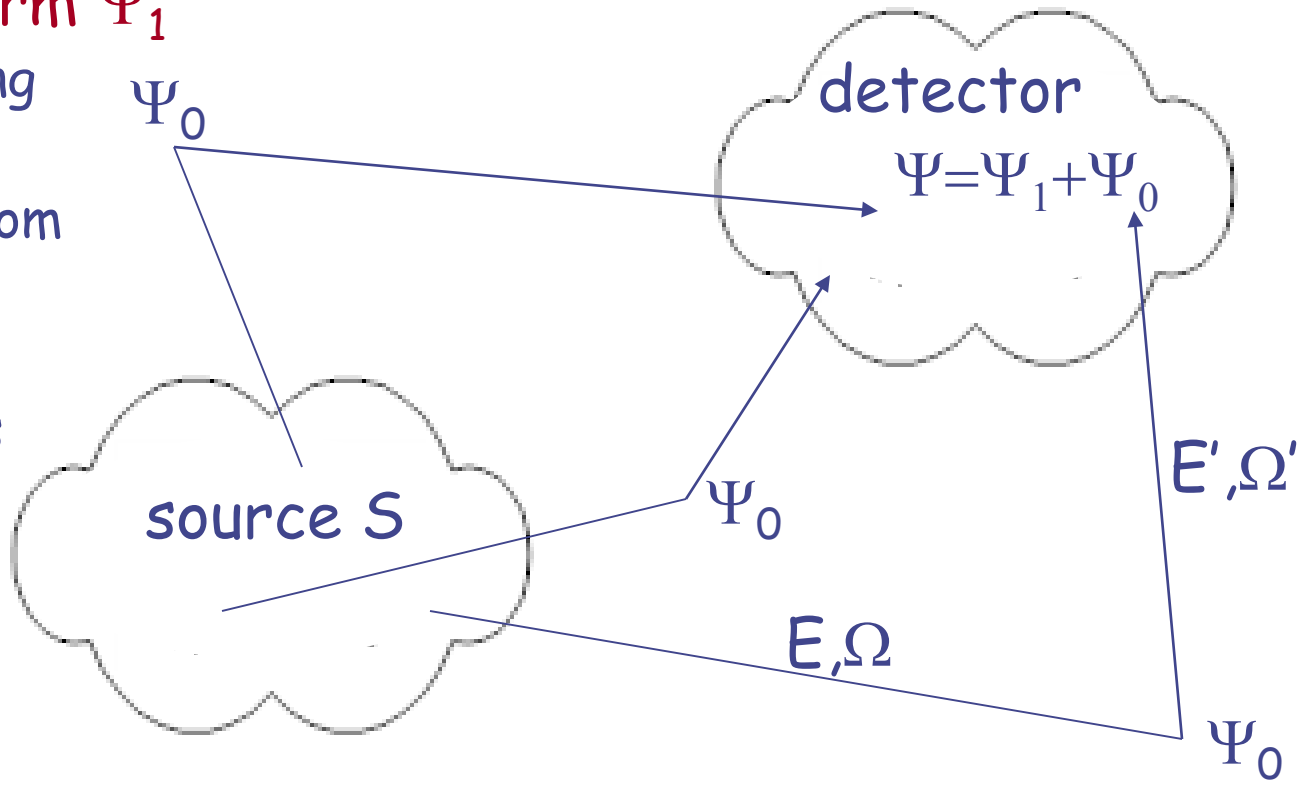
$e^{-\beta}$ = probability to reach detector without absorption nor scattering

"source" and "detector" are two regions of phase space

From source to detector with one scattering

once-collided term Ψ_1

obtained by summing (= integrating) all contributions from phase space points reached by uncollided particles



$$\Psi = \int_0^\infty e^{-\beta}\left[\iint_{E\Omega}\Sigma_s\Psi_0 d\vec{\Omega}dE\right]ds + Se^{-\beta} = \Psi_1 + \Psi_0 = K\Psi_0 + \Psi_0$$

(K: integral operator)

Neumann series

The solution of the Boltzmann equation in integral form is obtained by summing:

- the uncollided term Ψ_0
- the once-collided term $\Psi_1 = K\Psi_0$
- the twice-collided term $\Psi_2 = K\Psi_1$

etc...

Each term is derived from the previous one, adding one scattering

Neumann series:

$$\Psi_0 = Se^{-\beta}$$

$$\Psi_1 = K\,\Psi_0$$

$$\Psi_2 = K\,\Psi_1$$

.....

$$\Psi_n = K\,\Psi_{n-1}$$

Notice that analytical shielding formulae are written as:

$$D = D_0\, B(E)\, \mathrm{e}^{-\Sigma x}$$

where D (dose) is assumed to be proportional to Φ (fluence)

$D_0 e^{-\Sigma x}$ is the uncollided term

B (build-up factor) is the sum of all collided terms

Inverse sampling

Sampling from a generic continuous distribution:

- Integrate the distribution function, $f(x)$, analytically or numerically, and normalize to 1 to obtain the normalized cumulative distribution:

$$F(\xi) = \frac{\int_{x_{\min}}^{\xi} f(x)\,dx}{\int_{x_{\min}}^{x_{\max}} f(x)\,dx}$$

Again, we use the cumulative probability: remember, MC is integration!

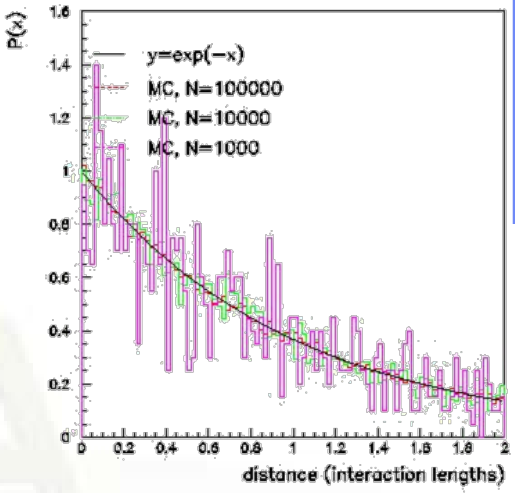
- Generate a uniform pseudo-random number ξ
- Get a sample of $f(x)$ by finding the inverse value $X = F^{-1}(\xi)$, analytically or most often numerically by interpolation (table look-up)
- Since ξ is uniformly random:

$$P(a \le x < b) = P[F(a) \le \xi < F(b)] = F(b) - F(a) = \int_a^b f(x)dx$$

Analytical sampling

Example: sampling from an exponential distribution (this is frequently needed in particle transport, to find the step length to the next interaction or the distance to decay)

$$f(x) = e^{-x/\lambda} \;,\; x \in [0,\infty)$$



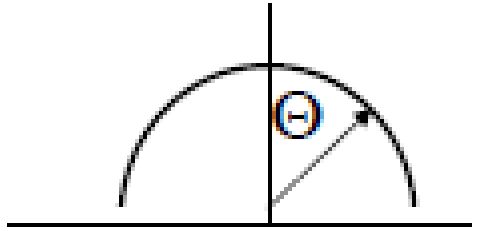
- Cumulative distribution: $F(t) = \int_0^t e^{-\frac{x}{\lambda}} dx = \lambda(1 - e^{-\frac{t}{\lambda}})$
- Normalized: $F'(t) = \int_0^t \frac{e^{-\frac{x}{\lambda}}}{\lambda} dx = 1 - e^{-\frac{t}{\lambda}}$
- Sample a uniform $\xi \in [0,1)$, e.g.: 0.745 $\quad \xi = F'(t) = 1 - e^{-\frac{t}{\lambda}} = 0.745$
- Sample t by inverting: $t = -\lambda \ln(1 - \xi)$
- But ξ is distributed like $1 - \xi$. Therefore our sampled value is:

$$t = -\lambda \ln \xi = -\lambda \ln 0.745 = 0.294 \lambda$$

- If we are sampling the next interaction point, we will make a step of 0.294 mfp

Sampling a uniform isotropic radiation field

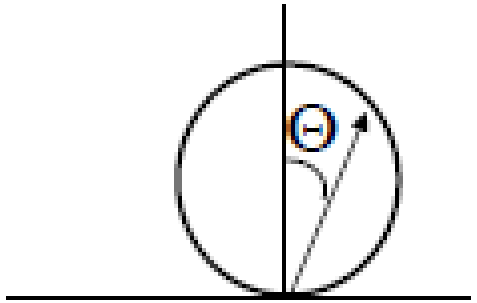
Several problems (e.g. concerning cosmic rays or phantom dosimetry require to simulate a uniform isotropic radiation field over a region of space



Uniform Distribution

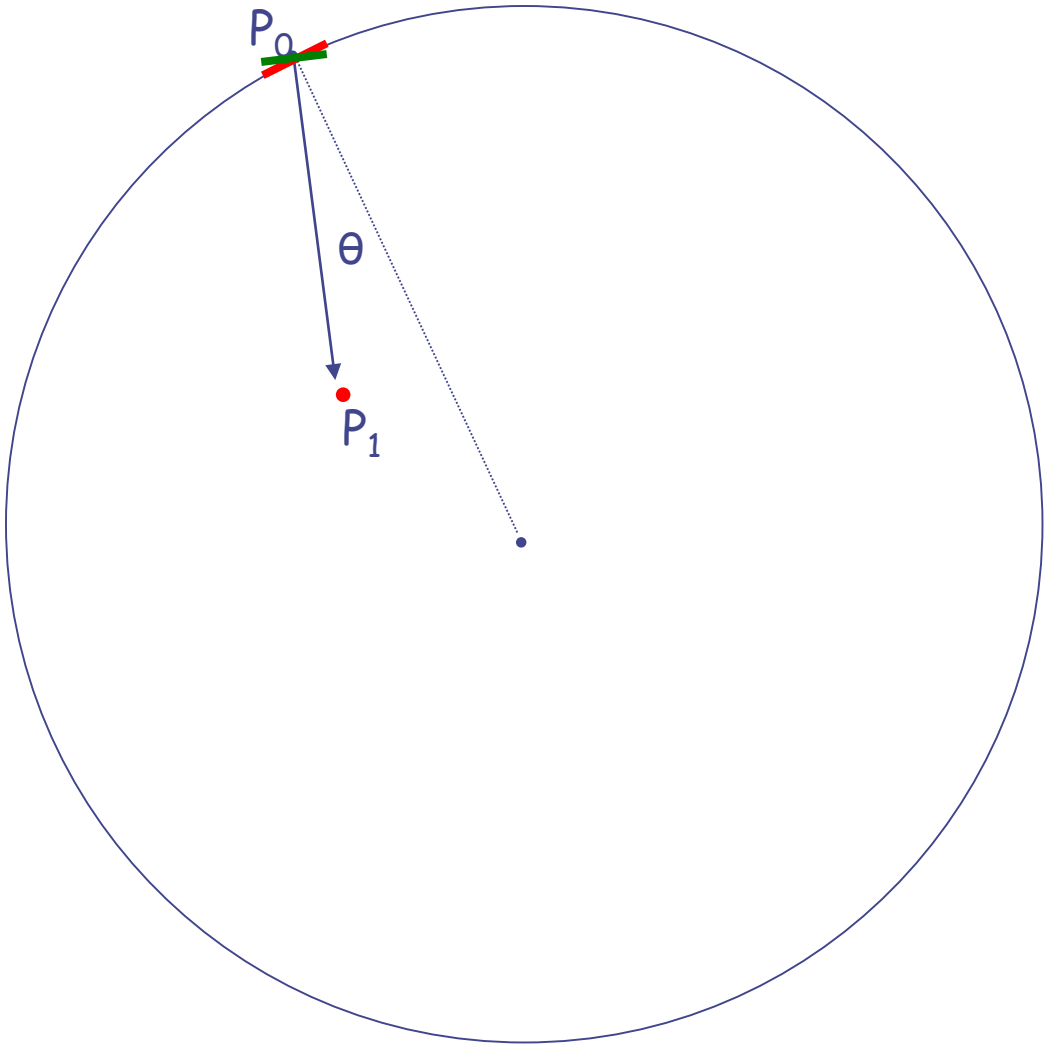
This can be obtained as follows:

- select a random point on the surface a sphere of radius R surrounding the region
- sample a random inward direction from a cosine distribution
- send the particle from point R in the selected direction



Cosine Distribution

Sampling a uniform isotropic radiation field



Why the cosine distribution?

The solid angle $d\Omega'$ subtended by the element of sphere surface at random point P_0 from a generic point P_1 is = $d\Omega \cos\theta$, where $d\Omega$ is the solid angle subtended in the direction of the normal in P_0

Cumulative distribution function

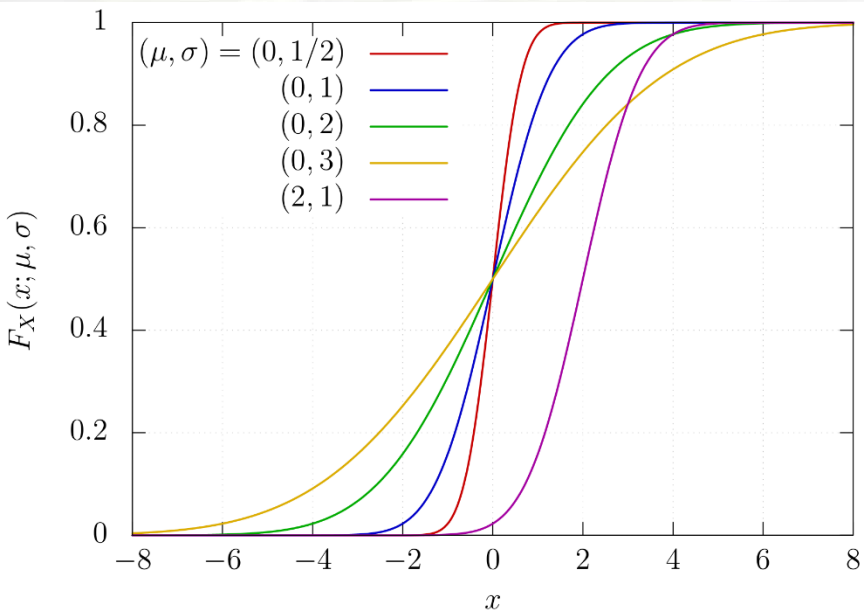
The cumulative distribution function F(x) describes the probability of obtaining a value smaller than x:

$$F(x) = \int_{-\infty}^{x} \mathrm{d}x'\; p(x')$$

It follows that:

- *F(-∞)=0*
- *F(∞)=1*
- *F(x) is a monotonically increasing function.*

Example: cumulative function of a Gaussian distribution:



Sampling from a distribution

Sampling from a discrete distribution:

Suppose we have a *discrete* random variable x, that can assume values $x_1, x_2, \ldots, x_n, \ldots$ with probability $p_1, p_2, \ldots, p_n, \ldots$

- Assume $\sum_i p_i = 1$, or normalize it
- Divide the interval [0,1) in n subintervals, with limits

$$y_0 = 0,\ y_1 = p_1,\ y_2 = p_1 + p_2, \ldots .$$

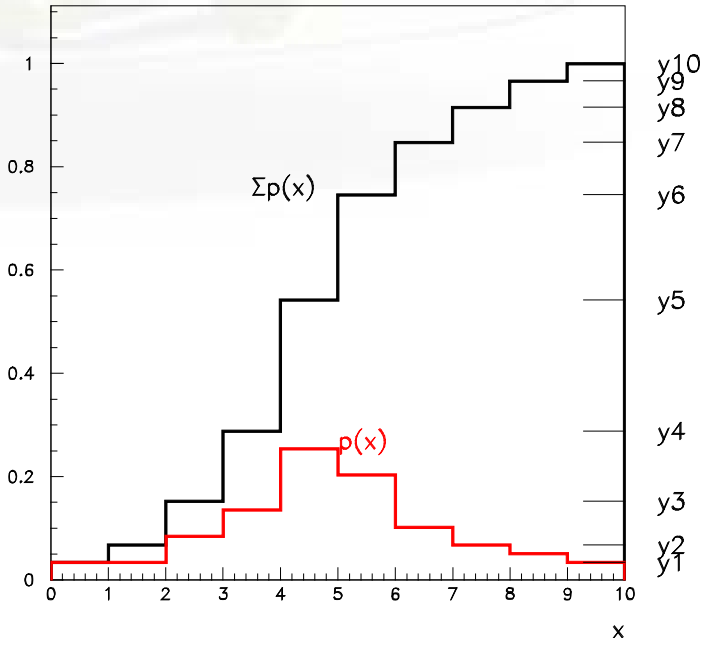
Note the use of the cumulative probability!

- Generate a uniform pseudo-random number $\xi \in [0,1[$
- Find the i^{th} y-interval such that

$$y_i - 1 \le \xi < y_i$$

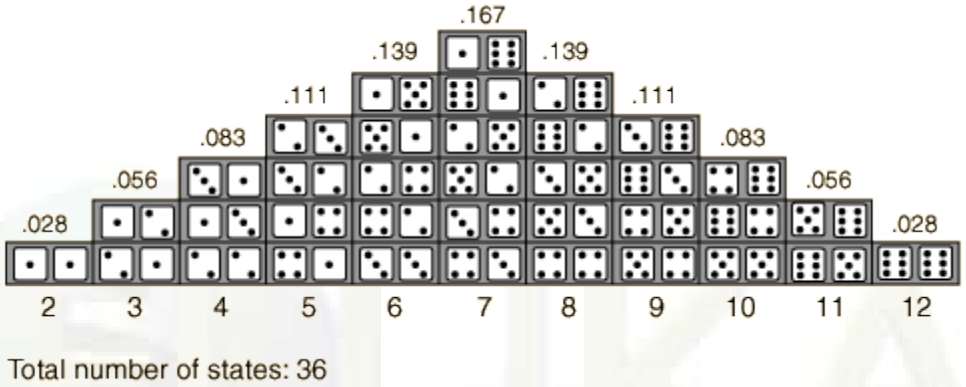
- Select $X = x_i$ as the sampled value
- Since ξ is uniformly random:

$$P(x_i) = P(y_{i-1} \le \xi < y_i) = y_i - y_{i-1} = p_i$$



Sampling from a distribution

Example: simulate a throw of dice 



$x_1 = 2, x_2 = 3, x_3 = 4, \ldots, x_{11} = 12$

$y_0 = 0, y_1 = 1, y_2 = 1+2 = 3, y_3 = 3+3 = 6, \ldots, y_{11} = 35+1 = 36$

Normalize:

$y_0 = 0, y_1 = 1/36 = 0.028, y_2 = 3/36 = 0.083, y_3 = 0.167, \ldots, y_{11} = 1$

Get a pseudorandom number ξ , e.g.: 0.125

ξ is found to be between $y_2 = 0.083$ and $y_3 = 0.194$

So, our sampled dice throw is $x_3 = 4$

Sampling from a distribution: the rejection technique

The rejection technique

- Some distributions cannot be easily sampled by integration and inversion (e.g. multi-dimensional or equation cannot be solved analytically)
- Let $f'(x)$ be one such distribution (normalized) that we want to sample
- Let $g'(x)$ be another normalized distribution function that can be sampled, such that $Cg'(x) \geq f'(x)$, for all $x \in [x_{min}, x_{max}]$
- Generate a uniform pseudo-random number $\xi_1 \in [0,1)$ to sample X from $g'(x)$
- Generate a second pseudo-random number ξ_2
- Accept X as a sample of $f'(x)$ if $\xi_2 < f'(X)/Cg'(x)$, otherwise re-sample ξ_1 and ξ_2

Sampling with the rejection technique

- The probability of X to be sampled from g′(x) is g′(X), the one that ξ_2 passes the test is f′(X)/Cg′(X) : therefore the probability to have X sampled and accepted is the product of probabilities g′(X) f′(X)/Cg′(X) = f′(X)/C
- The overall efficiency (probability accepted/rejected) is given by

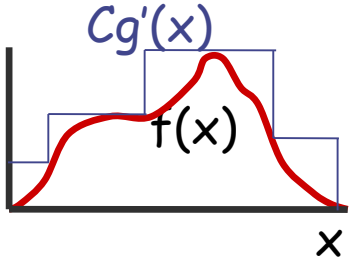
$$\varepsilon = \int \frac{f'(x)}{Cg'(x)} g'(x)dx = \int \frac{f'(x)}{C} dx = \frac{1}{C}\int f'(x)\,dx = \frac{1}{C}$$

f′(x) is normalized

- Proof that the sampling is unbiased (i.e. X is a correct sample from f′(x)): the probability P(X) dx of sampling X is given by:

$$P(X)\,dX = \frac{1}{\varepsilon} g'(X)\,\frac{f'(X)}{Cg'(X)}\,dX = f'(X)\,dX$$

- g′(X) is generally chosen as a uniform (rectangular) distribution or a normalized sum of uniform distributions (a piecewise constant function)



The rejection technique: example

Let be $f'(x) = (1+x^2)$, $x \in [-1,1]$

We choose $g'(x)$ to be constant, and:

$Cg'(x) = \max(f'(x)) = 2$

To normalize it:

$$\int_{-1}^{1} g'(x)\,dx = 1 \Rightarrow 2\,g'(x) = 1 \Rightarrow g'(x) = \frac{1}{2}$$

We obtain $C = 2/g'(x) = 4$

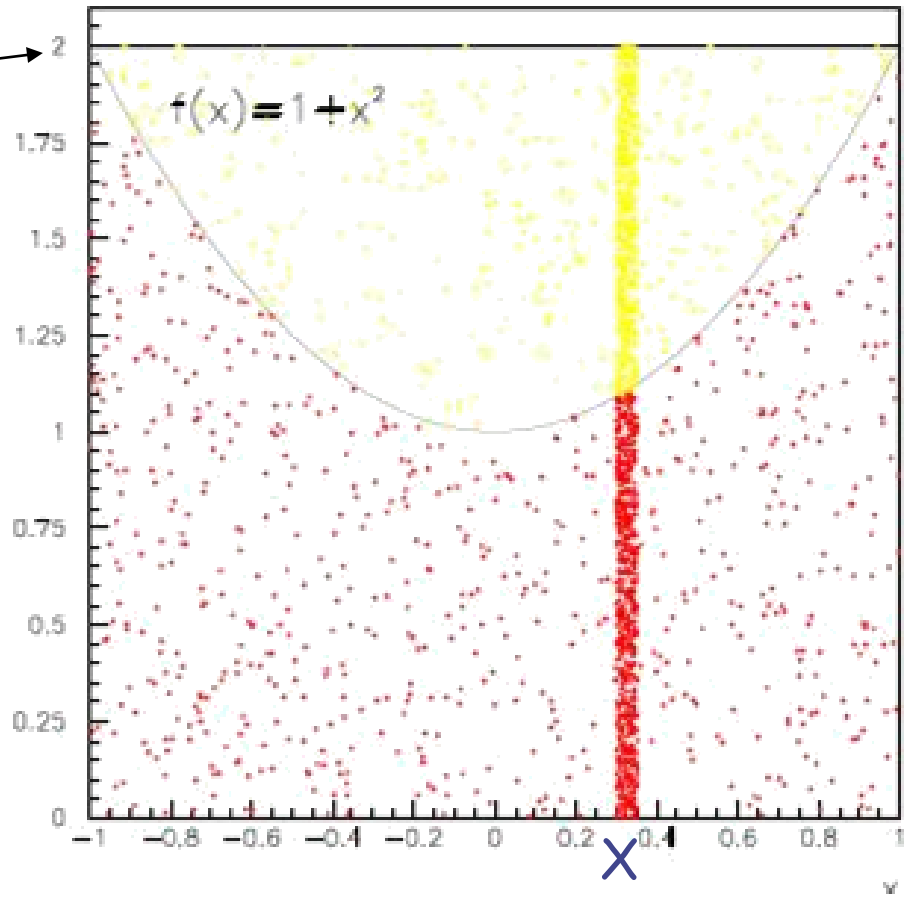
Generate two uniform pseudo-random numbers ξ_1, $\xi_2 \in [0,1)$

Sample X uniformly: $X = -1 + 2\xi_1$

Test:

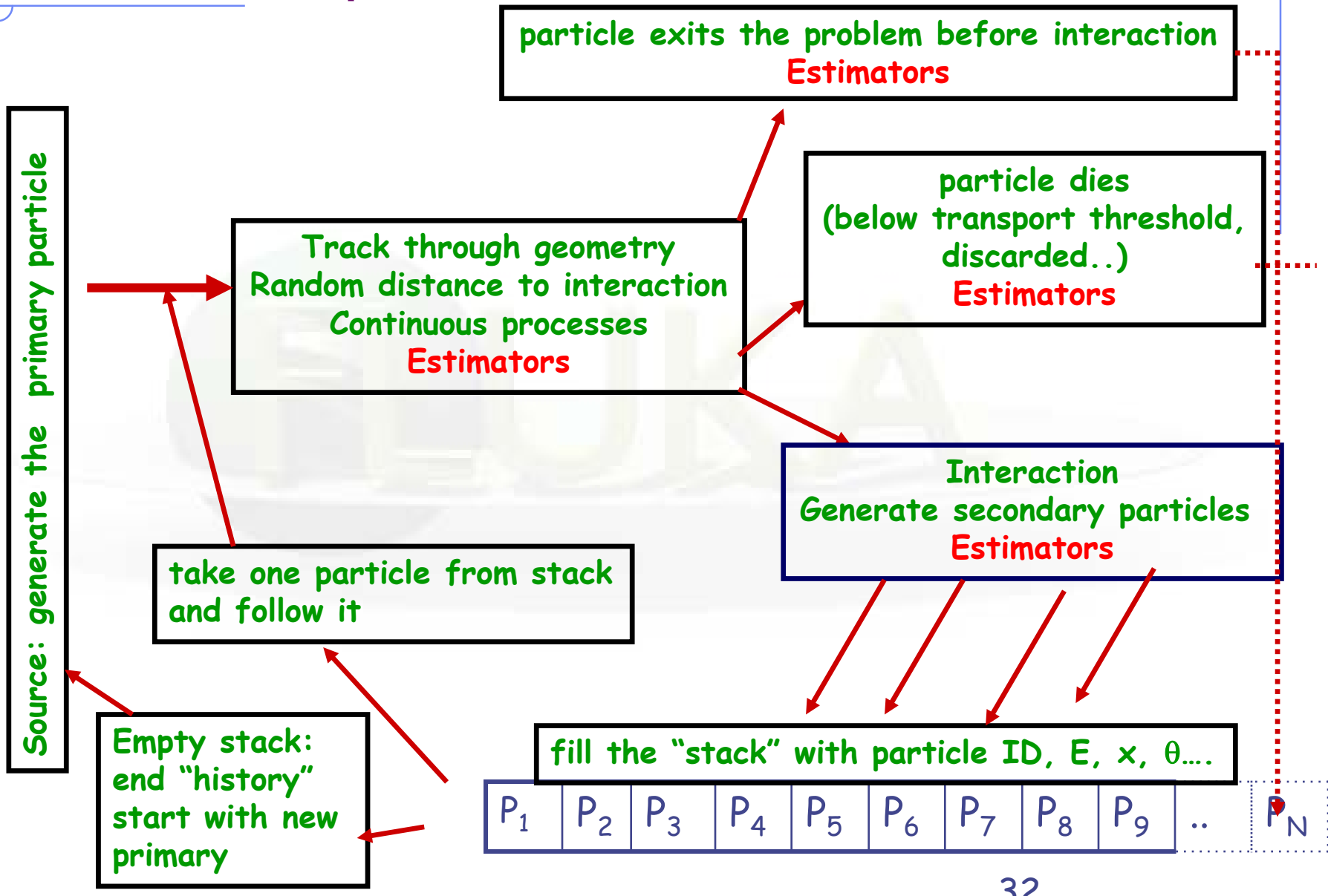
if $(1+X^2)/Cg'(x) = (1+X^2)/2 > \xi_2$, accept X

otherwise re-sample ξ_1, ξ_2



The efficiency is the ratio of the red area to the total

Practical implementations



Statistical errors, systematic errors, and… mistakes

Statistical errors, due to sampling (in)efficiency

Relative error	Quality of Tally *(from an old version of the MCNP Manual)*
50 to 100%	Garbage
20 to 50%	Factor of a few
10 to 20	Questionable
< 10%	Generally reliable

- Why does a 30% σ mean an uncertainty of a "factor of a few"? Because σ in fact corresponds to the sum (in quadrature) of two uncertainties: one due to the fraction of histories which don't give a zero contribution, and one which reflects the spread of the non-zero contributions
- The MCNP guideline is empirically based on experience, not on a mathematical proof. But it has been generally confirmed also working with other codes
- Small penetrations and cracks are very difficult to handle by MC, because the "detector" is too small and too few non-zero contributions can be sampled, even by biasing